

**STOICHIOMETRY MEASUREMENTS FOR THE PARAMETERIZATION OF  
ABSOLUTE RATE MODELS FOR CYTOCHROME P450 METABOLISM**

ABSTRACT OF THE DISCLOSURE

5        Systems and method are provided for modeling substrate molecules so that the various pathway reaction rates, and thus their overall reaction rates and metabolic properties, can be predicted. The current invention provides various systems and methods for stoichiometrically measuring the pathway reaction rates, both directly and indirectly. By repeating this for a class or several classes of substrate molecules, a  
10      general model of pathway reaction rates can be developed by correlating observed pathway reaction rates to the actual structural descriptors of the molecules, in particular, features around the reactive sites. The model can then be used to predict and design substrates according to desired metabolic characteristics. The systems and methods are particularly applicable to metabolism of substrate molecules by the cytochrome P450  
15      enzymes.